LA-UR-21-24698

Title: Nonlinear problems in THC Salt simulations

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Intended for: Program review

Issued: 2021-05-14

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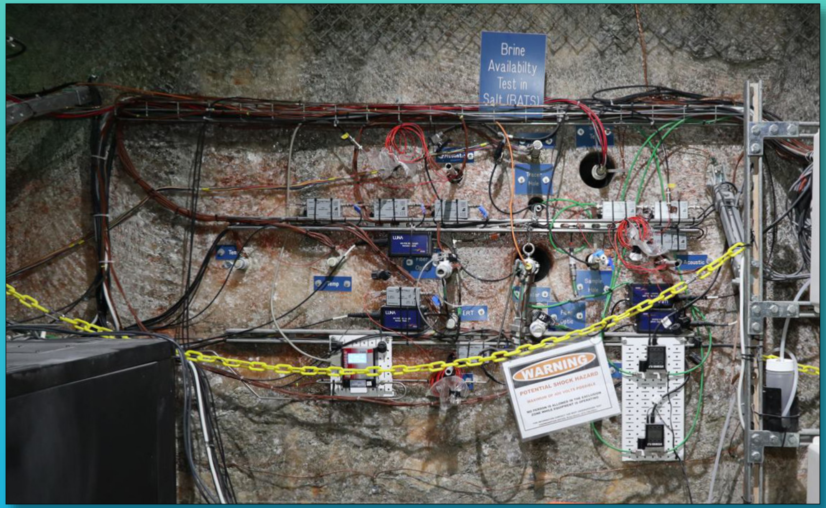
Spent Fuel and Waste Science and Technology (SFWST)

Clean. Reliable. Nuclear.

Cross-Cut: Nonlinear Problems in Repository Science



Lightning Talk : Nonlinear problems in THC Salt simulations

SFWST Annual Meeting

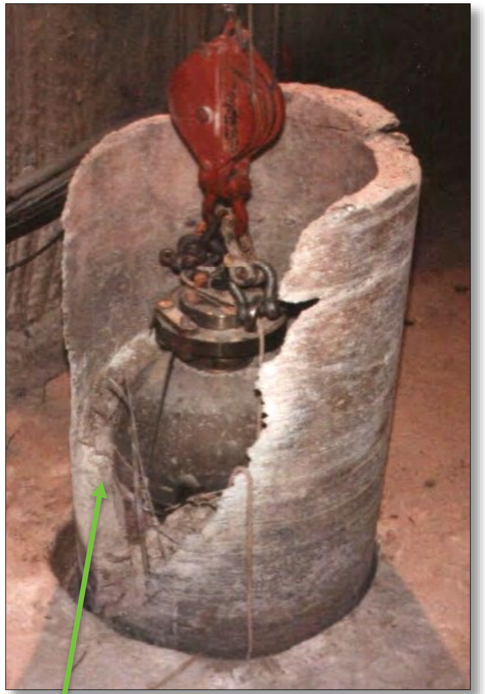
Tuesday May 18, 2021 (11:00-12:30)

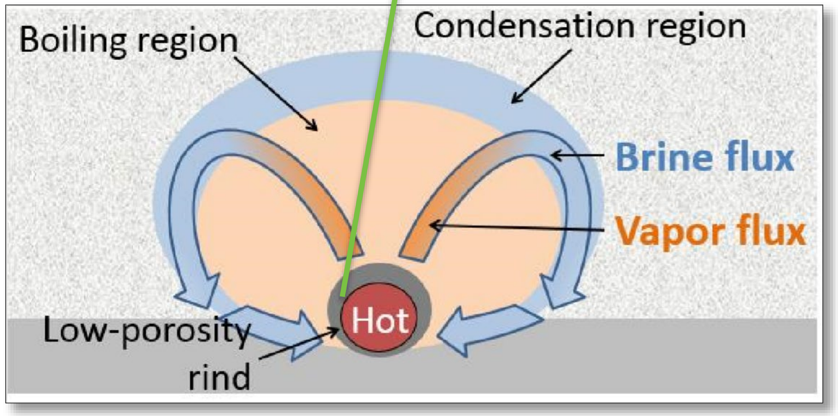
Philip H. Stauffer

Los Alamos NATIONAL LABORATORY

What problems do we have modeling heated salt?

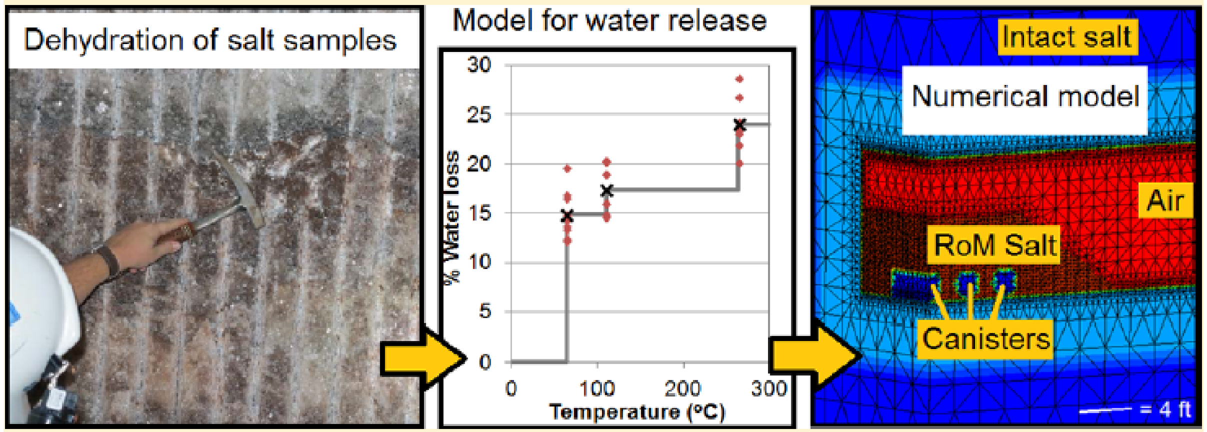
- Salt is "thermally activated"
  - High temperatures speed up creep closure
  - More brine available in hot salt
  - Salt more soluble in hot brine
- High temperatures lead to dry-out
  - Water driven off as vapor, forming salt crust
  - Near-package permeability reduced
  - Less corrosion in dry environment
- Coupled models (Δ porosity / permeability)
  - Creep, damage & healing
  - Precipitation & dissolution
  - Brine migration (rel. permeability)
    - Gas-filled fractures
    - Liquid-saturated far field

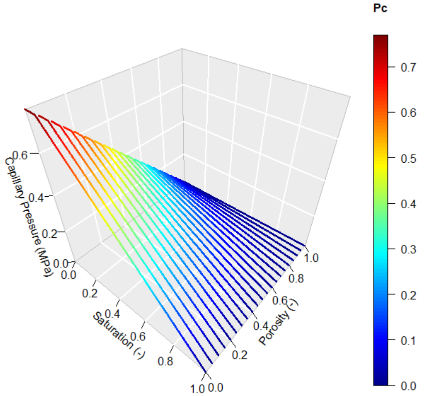




Salt THMC Couplings

Deformation (strain)	***F***(*stress, time, saturation, temperature*)
Vapor pressure lowering	***F***(*capillary pressure, salinity*)
Porosity	***F***(*dissolution, precipitation, stress, strain*)
Thermal conductivity	***F***(*porosity, saturation, temperature*)
Permeability	***F***(*dissolution, precipitation, porosity, saturation*)
Capillary pressure	***F***(*porosity, saturation, temperature*)
Water vapor diffusion	***F***(*porosity, saturation, temperature*)
Clay dehydration	***F***(*temperature*)
Salinity	***F***(*temperature*)

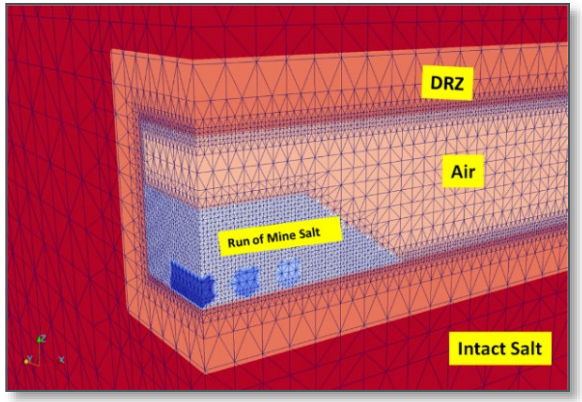




Capillary pressure / porosity function

THMC Process-Level Modeling

- Thermal-Hydrological-Mechanical-Chemical (THMC)
- TOUGH-FLAC simulates large-deformation THMC
- FEHM + PFLOTRAN numerical models simulates small-deformation THMC
- Isolating specific processes allows more rapid validation
- Some processes are validated using TH, TM, THC, or THM




Example 1

As liquid water disappears by evaporation/boiling, there is a disconnect in the governing equations

FIX: requires variable switching

Can cause oscillations around

0 saturation in the solver.

Phases state	Primary variables
Full water saturation	Pressure, Temperature
2-phase, 100% relative humidity	Pressure, Temperature, Saturation
Zero saturation (steam/air)	Pressure, Temperature, Air Mass Fraction

In Phase state 3 when water vapor pressure goes to zero (dry air), big problems.

FIX: Extend the lookup table to zero water vapor pressure, with derivatives. Density ideal gas, enthalpy is a Taylor expansion, same with viscosity.

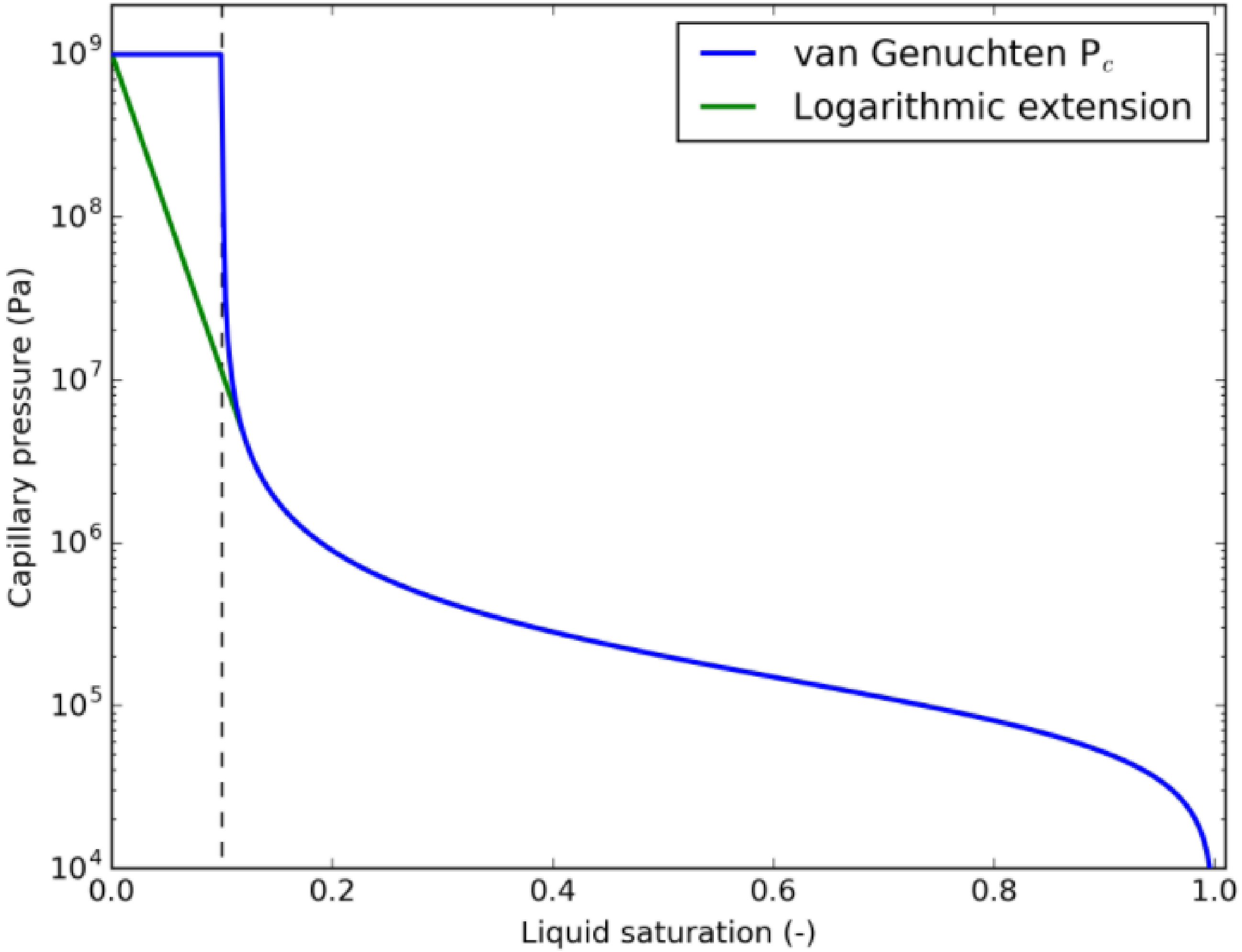
Could have: P T Total mass fraction(accumulation term of the non-condensables). SINGLE SET OF VARIABLE

Example 2

When approaching dry-out, the capillary suction is highly non-linear

Fix: Modify the tail of the function at low saturation

- Linear or logarithmic
- Allows the function to go past the 'residual saturation'
- User can control maximum capillary pressure



https://mooseframework.inl.gov/modules/porous_flow/capillary_pressure.html

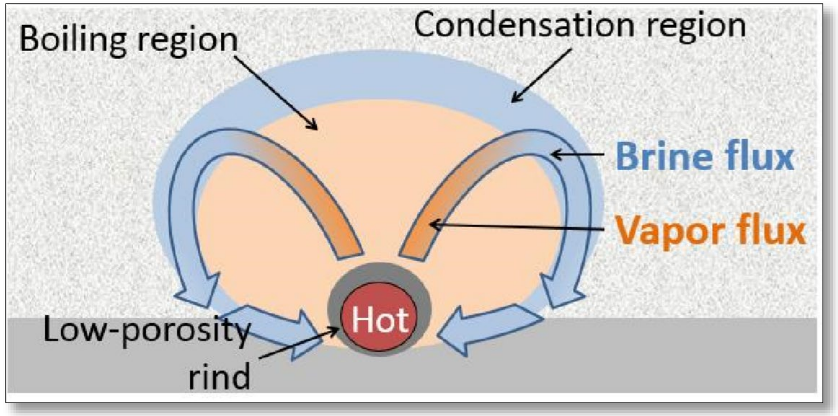
Example 3 – work in progress

As dry-out happens, concentrations in the liquid can go crazy.

Fix: For non-vapor species, make sure solubility goes to zero, so that chemical turns solid as the water disappears.

For vapor species like O18 and D, there must be a similar trick to ensure that all the tracer is gone before the last water leaves the liquid state, otherwise concentration can go wild.

Fix, if total tracer mass goes below some tolerance, report zero (or below tolerance), might compare to previous time step.



Next: More Lightning Talks